Isopropyl beta-D-1-thiogalactopyranoside
367-93-1 | DTXSID6041052

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: -1.16

Global applicability domain: Inside

Local applicability domain index: 6.83e-01

Confidence level: 6.63e-01

Nearest Neighbors from the Training Set

Image not found
Isopropyl beta-D-1-
thiogalactopyranoside
Measured: -1.26
Predicted: -1.16

Image not found
Ethyl 1-thio-beta-D-
galactopyranoside
Measured: -1.51
Predicted: -1.31

Image not found
NSC226971
Measured: -0.630
Predicted: -0.623

Image not found
Dibromomannitol
Measured: -0.240
Predicted: -0.498

Image not found
Dibromodulcitol
Measured: -0.240
Predicted: -0.498